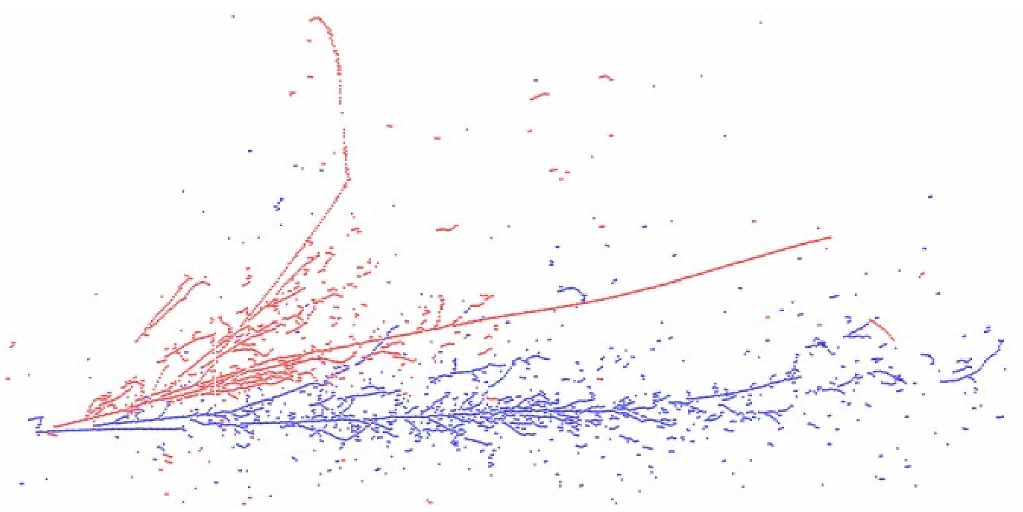
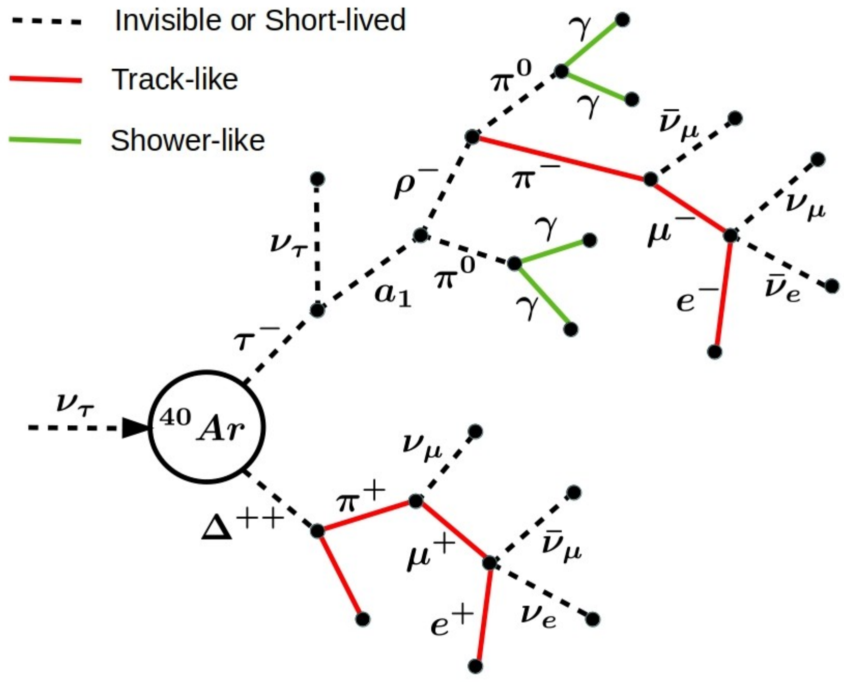
A Multipurpose Graph Neural Network for Reconstruction in LArTPC Detectors





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NNN23
Procida, Italy
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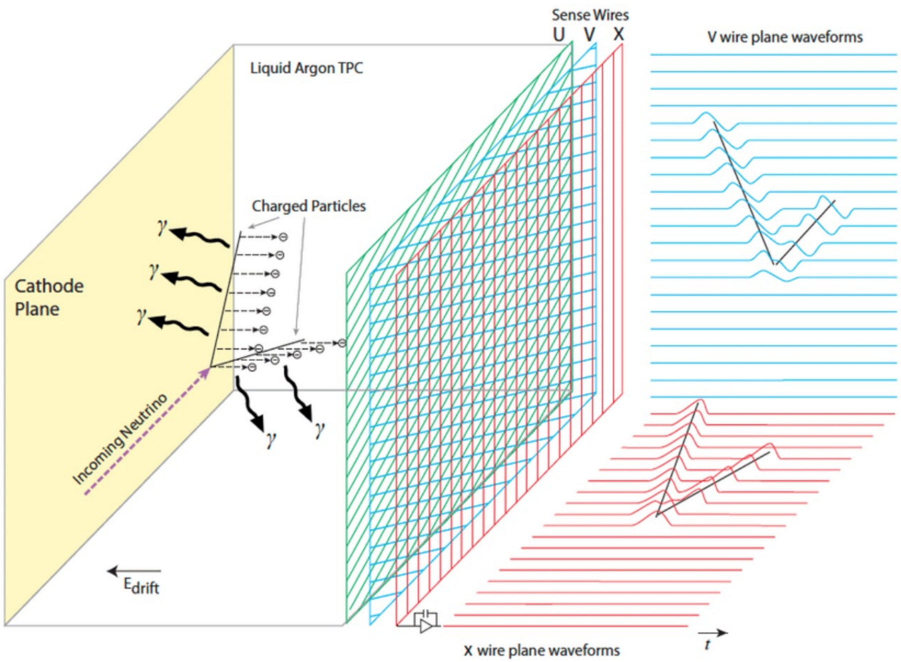
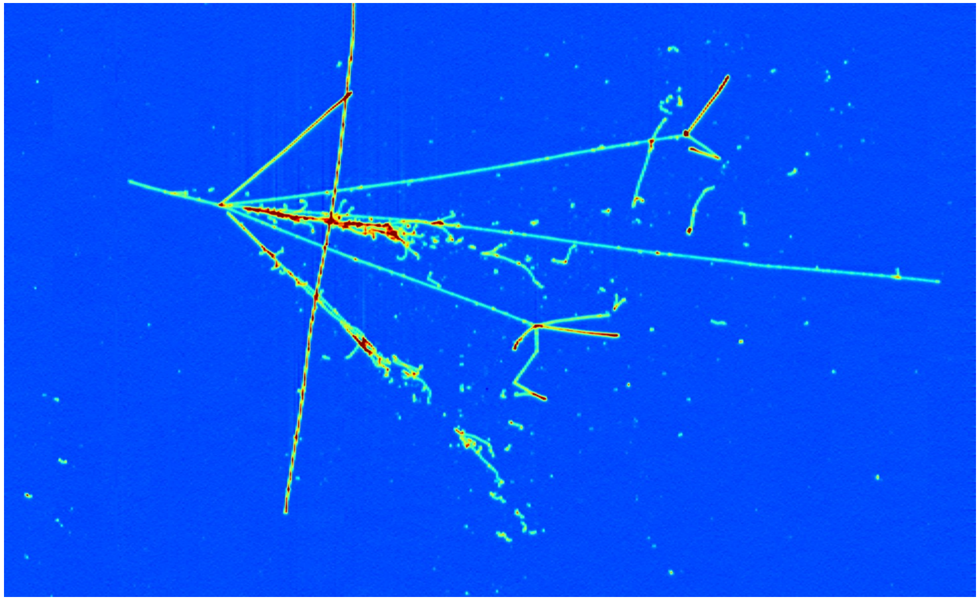
Liquid Argon Time Projection Chambers



- LArTPCs are currently heavily used in neutrino physics
  - Now: MicroBooNE, Icarus, SBND
  - Future: DUNE (70 kT far detector deep underground)
- Charged particles ionize liquid argon as the travel
- Ionization electrons drift due potential between cathode and anode planes
- Closely spaced wires (~3 mm) at anode provide high-resolution image of neutrino interaction
- Multiple wire planes provide 3D information

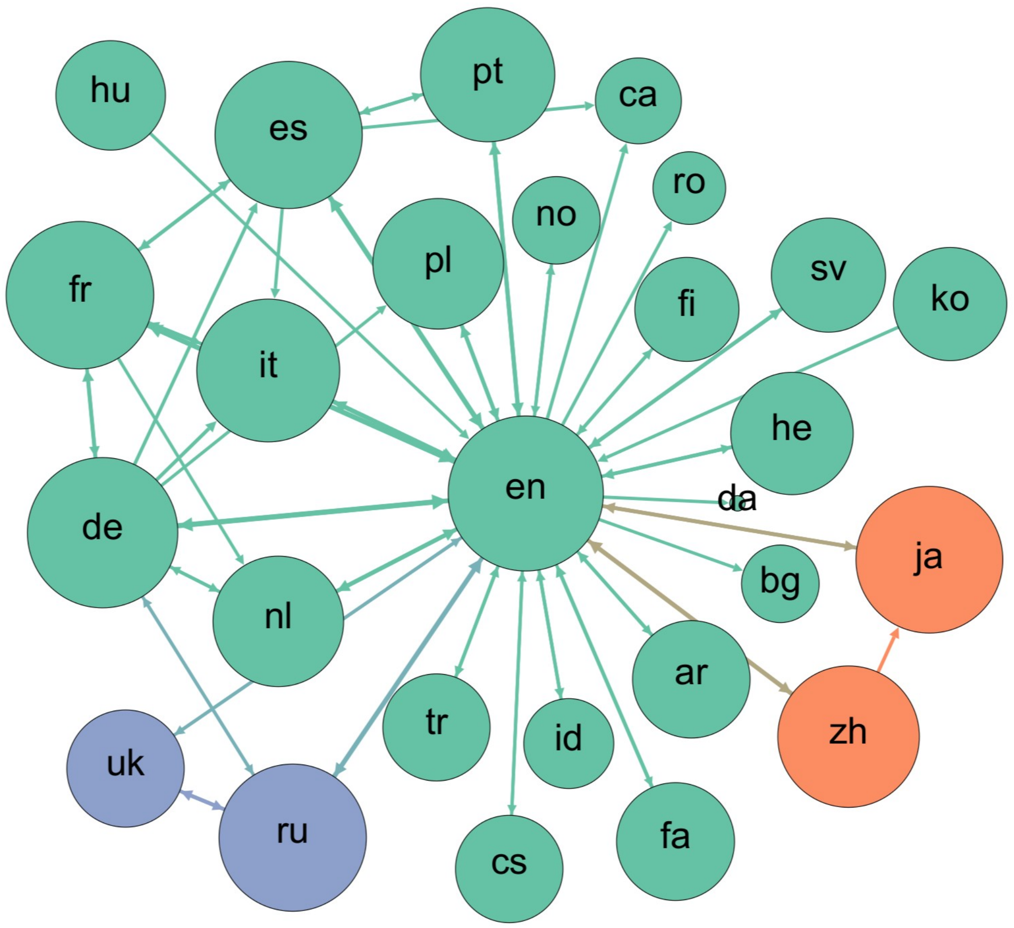
- High resolution images are blessing and curse
- Would like to
  - Cluster hits into objects
  - Classify objects according to the particle that created it
  - Assemble the objects into an event
  - Determine type and kinematic properties of the event



Graphs

- A graph is a mathematical structure that represents objects and binary relationships between them
  - Nodes: represent objects
    - Can hold associated information like spatial or temporal coordinates, or other features
  - Edges: connections between nodes
    - Relationship can be directed or undirected
    - Can have associated features
- Ideal structure for understanding physics data
  - Naturally sparse
  - Hits have a causal structure that can easily be modeled by edges
  - Accommodates relationships beyond nearest neighbor

$$G = (V, E)$$



From arXiv:1312.0976
Graph of Wikipedia editors who primarily edit in one language, but sometimes edit in another

Graph Neural Networks

- GNNs are an extension of the idea of CNNs
  - Instead of extracting features from patches in a regular grid, extract features from neighbors of node
- Iteratively learn a smart embedding of graph structure
- Encode geometric information by passing and aggregating messages from neighbors

Initial embeddings = node features

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

Average of neighbors' previous embeddings

Previous embedding of v

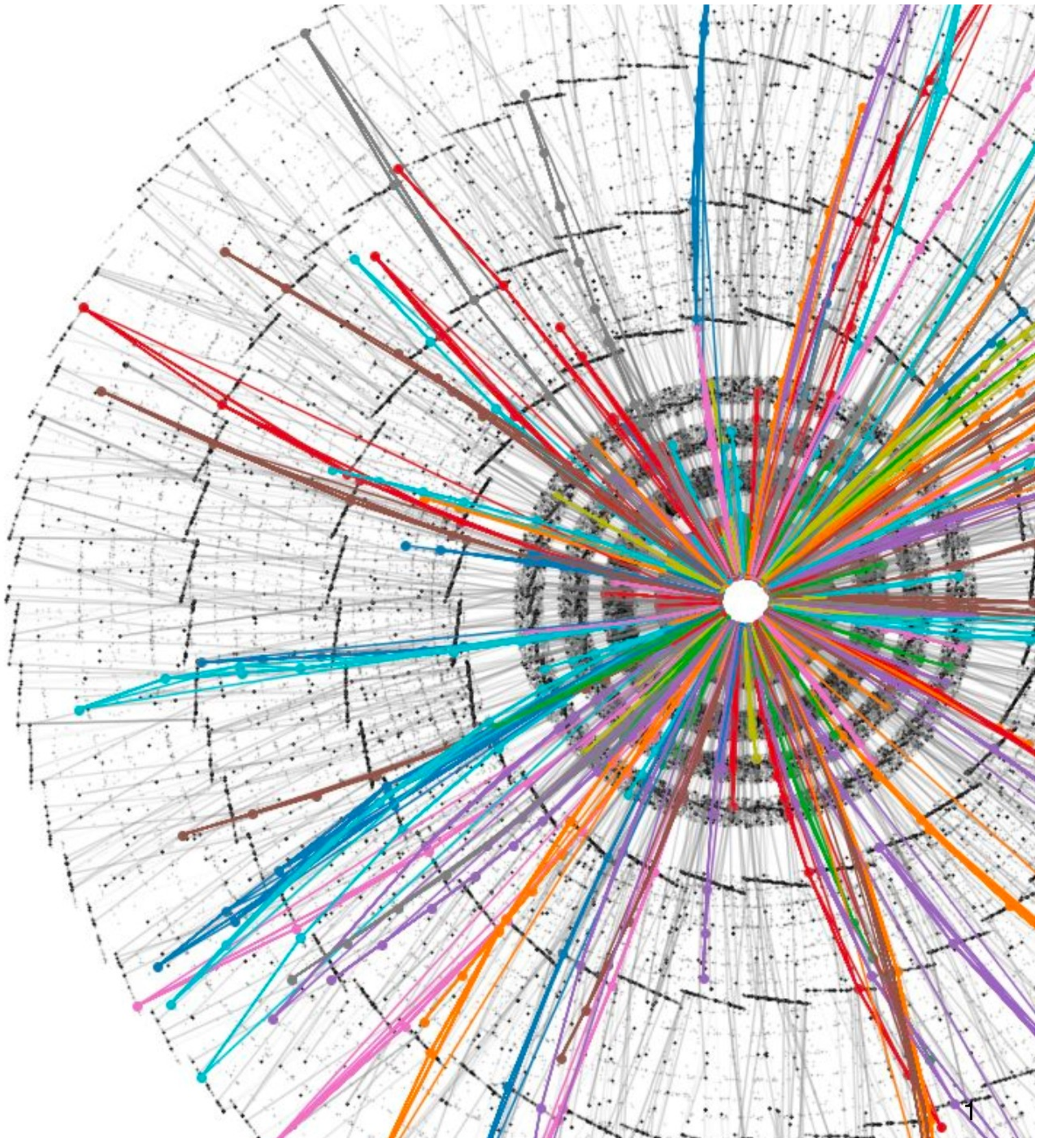
$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \forall k > 0$$

New embedding

Shallow neural networks

Exa.TrkX

- Exa.TrkX is a collaboration developing next-generation GNNs for HEP reconstruction
- Energy Frontier
  - Expand on HEP.TrkX's prototype GNN for HL-LHC tracking
  - Incorporate into ATLAS's simulation and validation chain
- Intensity Frontier
  - Explore viability of HEP.TrkX network for neutrino physics
  - Develop GNN-based reconstruction for LArTPCs



GNN Reconstruction for Neutrino Physics

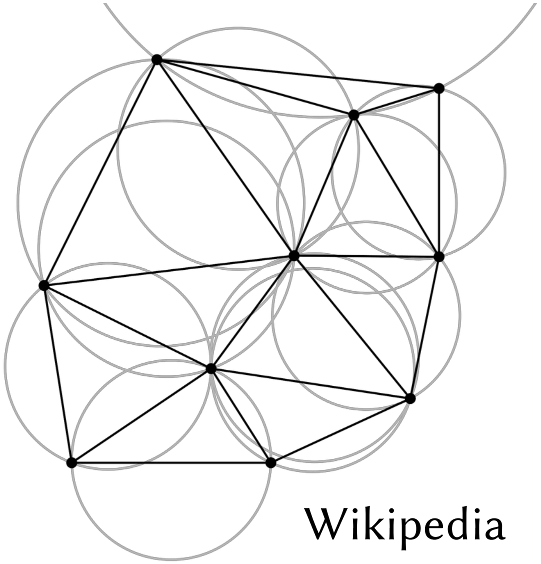
- This work uses simulated neutrino interactions from MicroBooNE's Open Data Release (link)
  - Simulated response of MicroBooNE detector to neutrino interactions with cosmic data overlays
    - Realistic simulation with detector imperfections modeled
- Network architecture was originally developed in the context of the DUNE far detector
  - Toward full reconstruction of high multiplicity atmospheric and ν_τ interactions
- Architecture is designed to have broad applicability
  - Currently deploying even on non-LArTPC experiments

Hit Classification

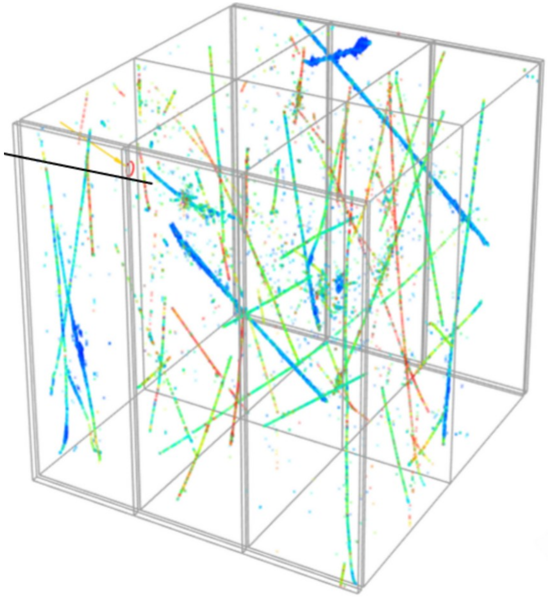
- The primary goal of NuGraph2 is to classify each detector hit according to particle type
- Five semantic categories:
  - MIP: minimum ionizing particles (muons, pions)
  - HIP: highly ionizing particles (protons, nucleons, kaons)
  - EM showers
  - Michel electrons
  - Diffuse activity (Compton scatters, neutrons)

Initial Event Graphs

- Message-passing algorithm requires constructing an initial graph out of the data
- MicroBooNE has three wire planes, so we construct three independent 2D graphs
  - Each node represents a reconstructed hit
    - Input features: wire index, hit time, integral, RMS width
  - Edges are formed for each 2D graph using Delaunay triangularization
    - Natively sparse representation
    - Both long and short distance edges for good information flow
- 3D hits can be formed by looking for coincidences between hits on three wire planes
  - 3D hits provide a way to connect three independent graphs together



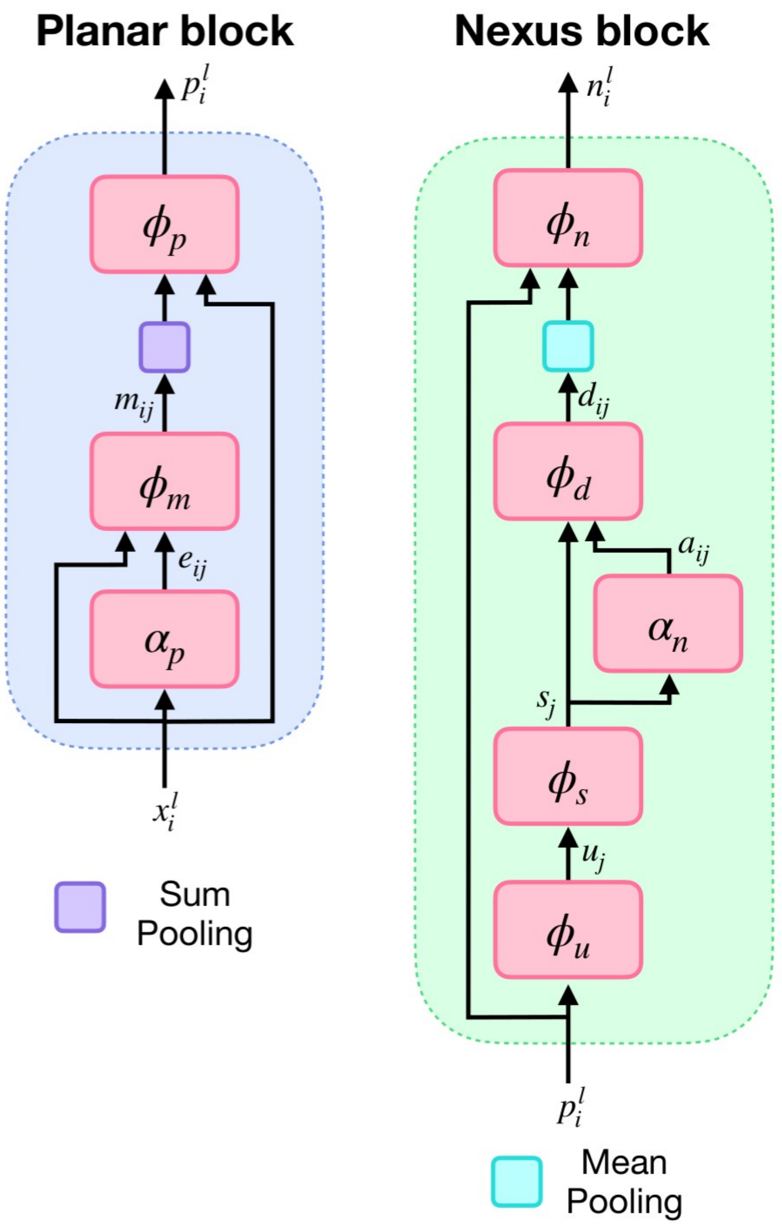
Wikipedia



arXiv:2002.03005

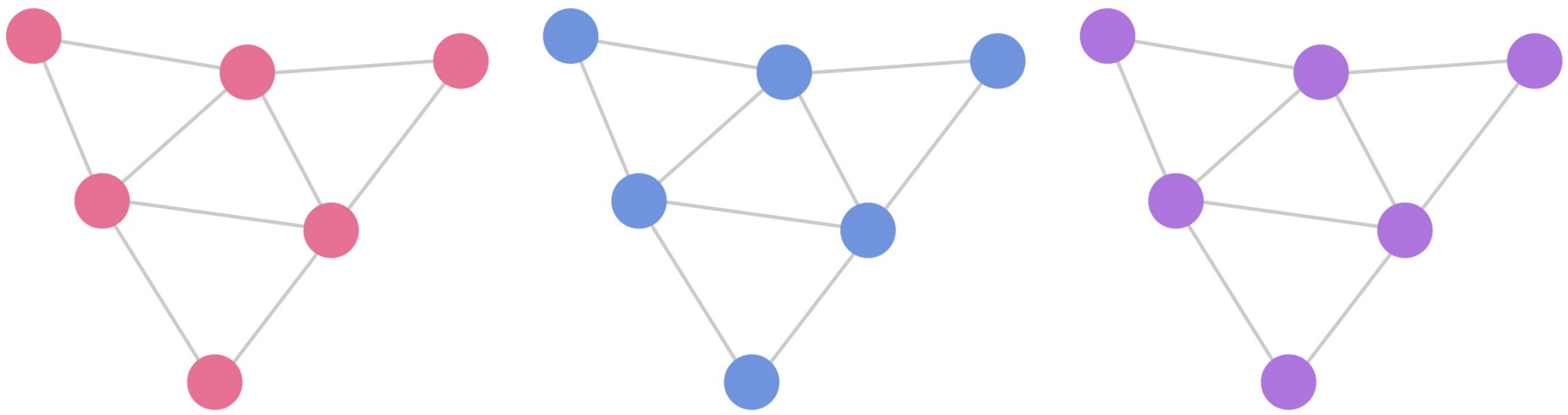
NuGraph2 Network Architecture

- NuGraph2's core convolution engine is a self-attention message passing network utilizing a categorical embedding
  - Each particle category is provided with a separate set of embedded features, which are convolved independently
  - Context information is exchanged between particle types via a categorical cross-attention mechanism
- Each message-passing iteration consists of two phases, the planar step and the nexus step:
  - Pass messages internally in each plane
  - Pass messages up to 3D nexus nodes to share information



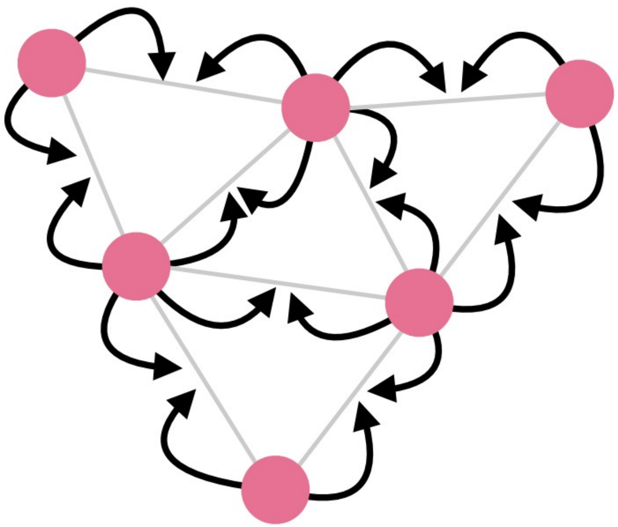
Message Passing Iteration Through the Graph

- Input graph three planar graphs with node features



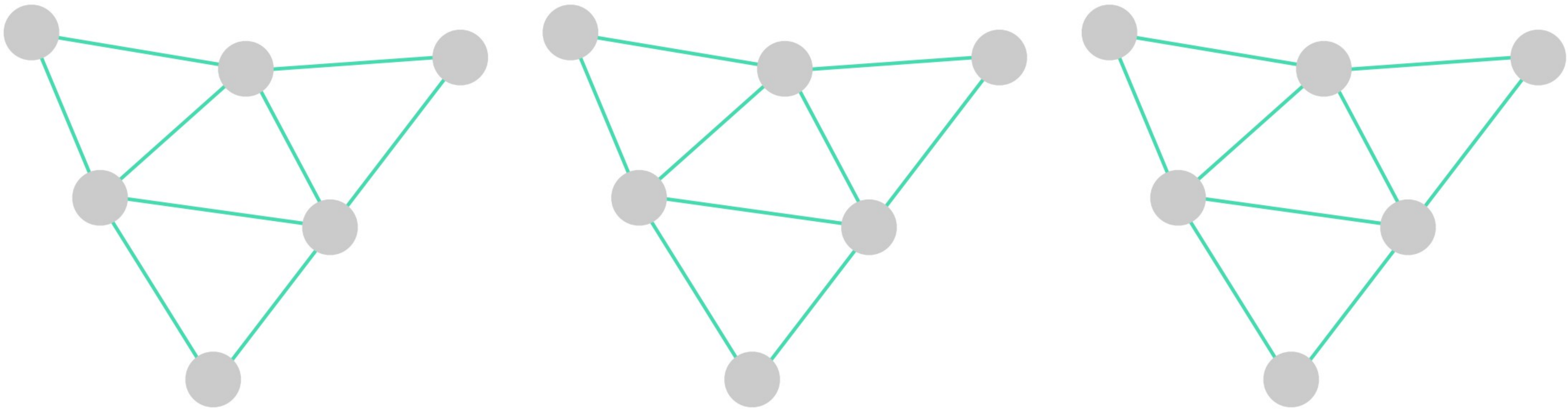
Message Passing Iteration Through the Graph

- Convolve node features to obtain edge features



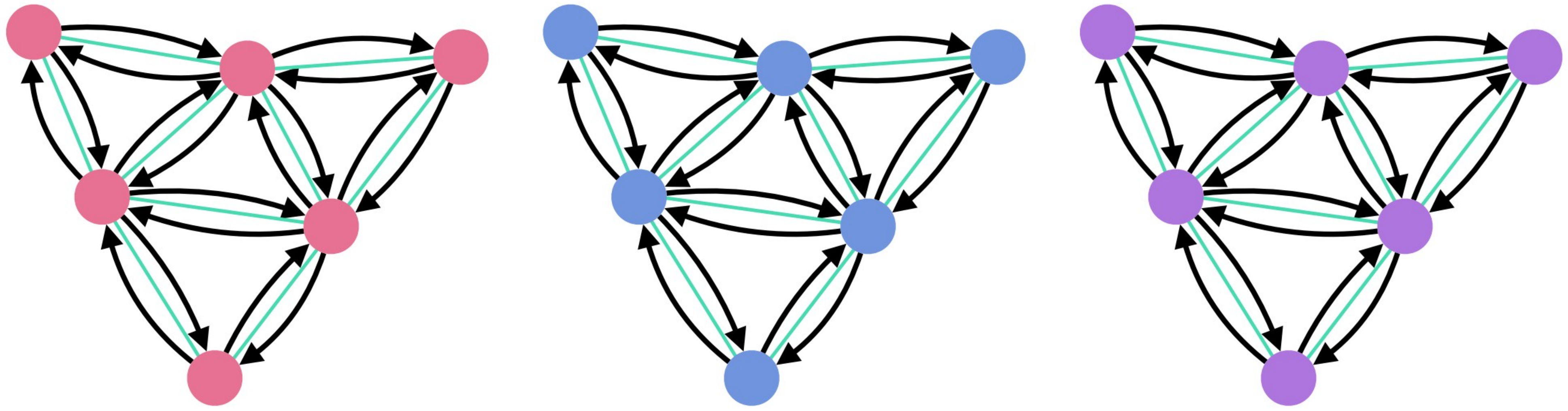
Message Passing Iteration Through the Graph

- Derive edge weights from edge features



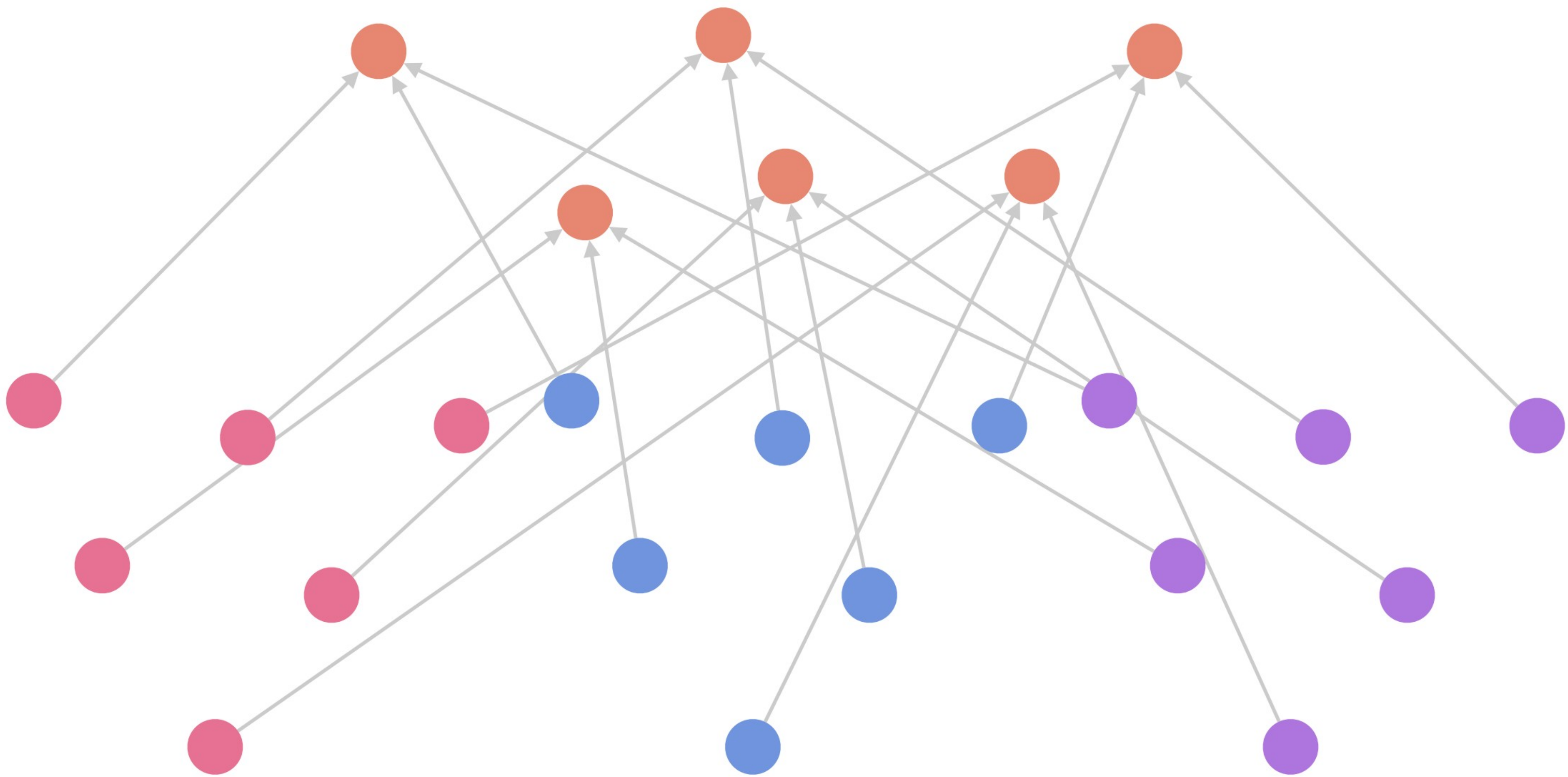
Message Passing Iteration Through the Graph

- Update node features using edge-weighted features from connected nodes



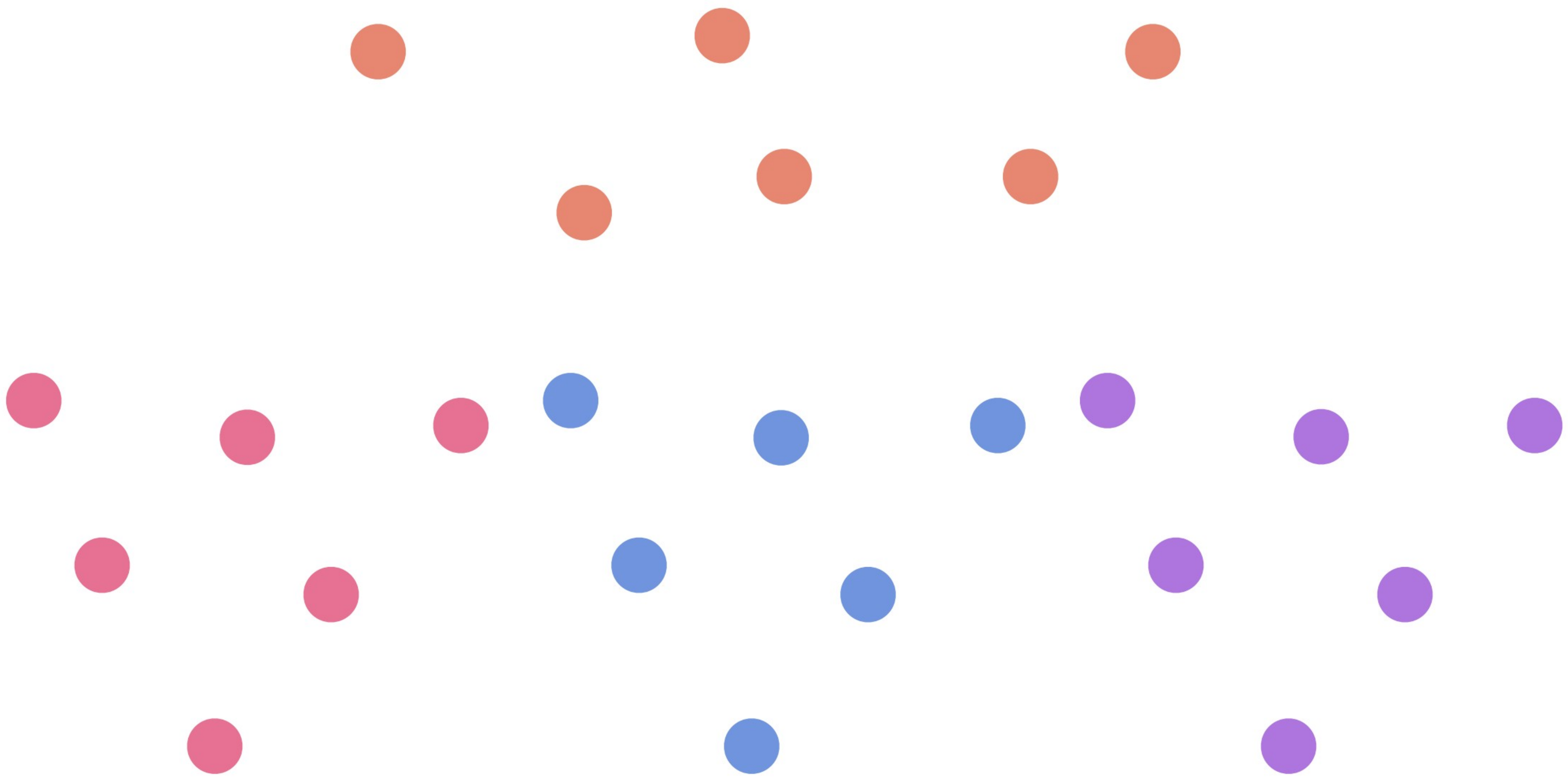
Message Passing Iteration Through the Graph

- Propagate node features to 3D nexus nodes



Message Passing Iteration Through the Graph

- Convolve nexus node features to mix information between planes



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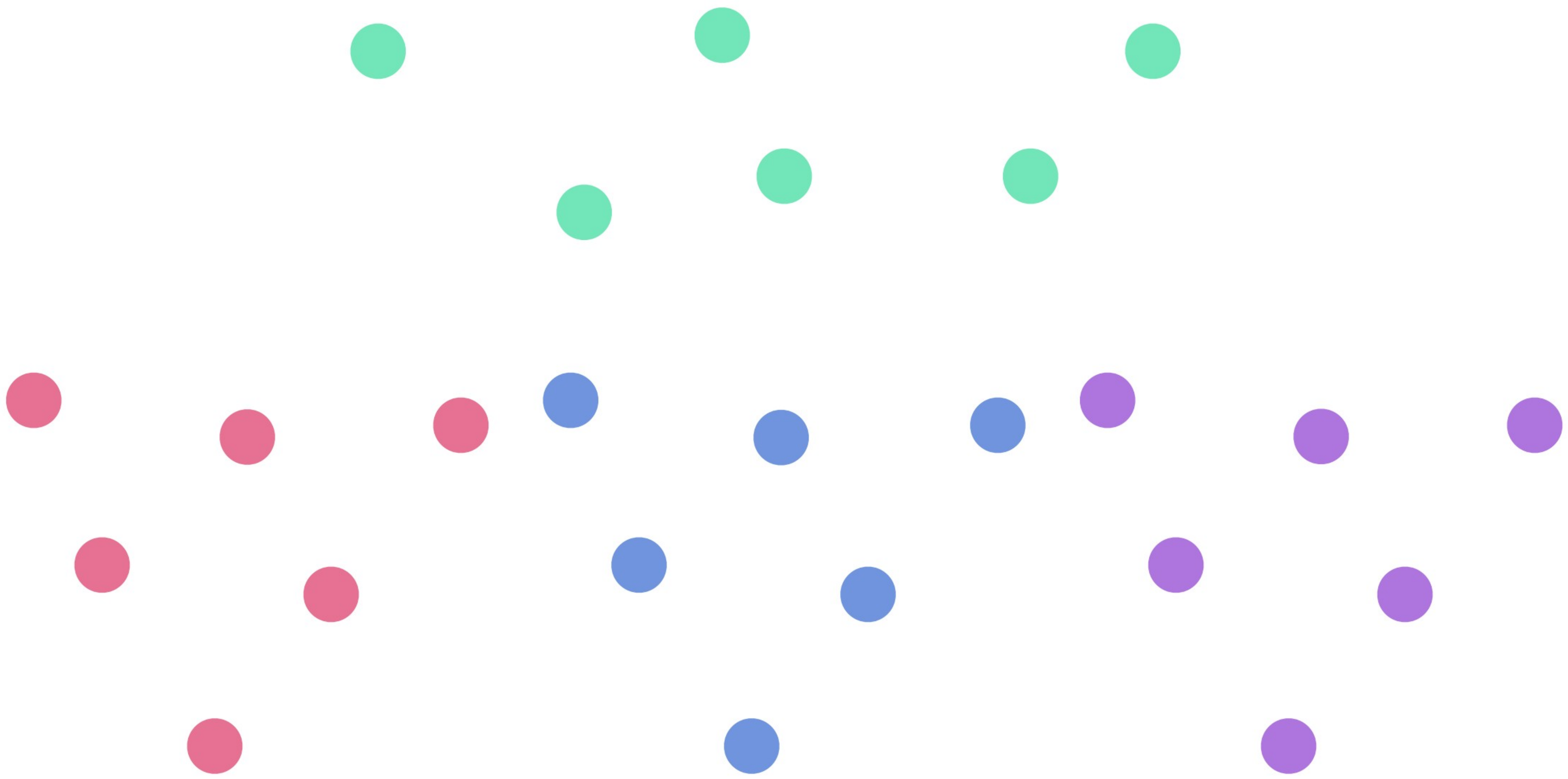
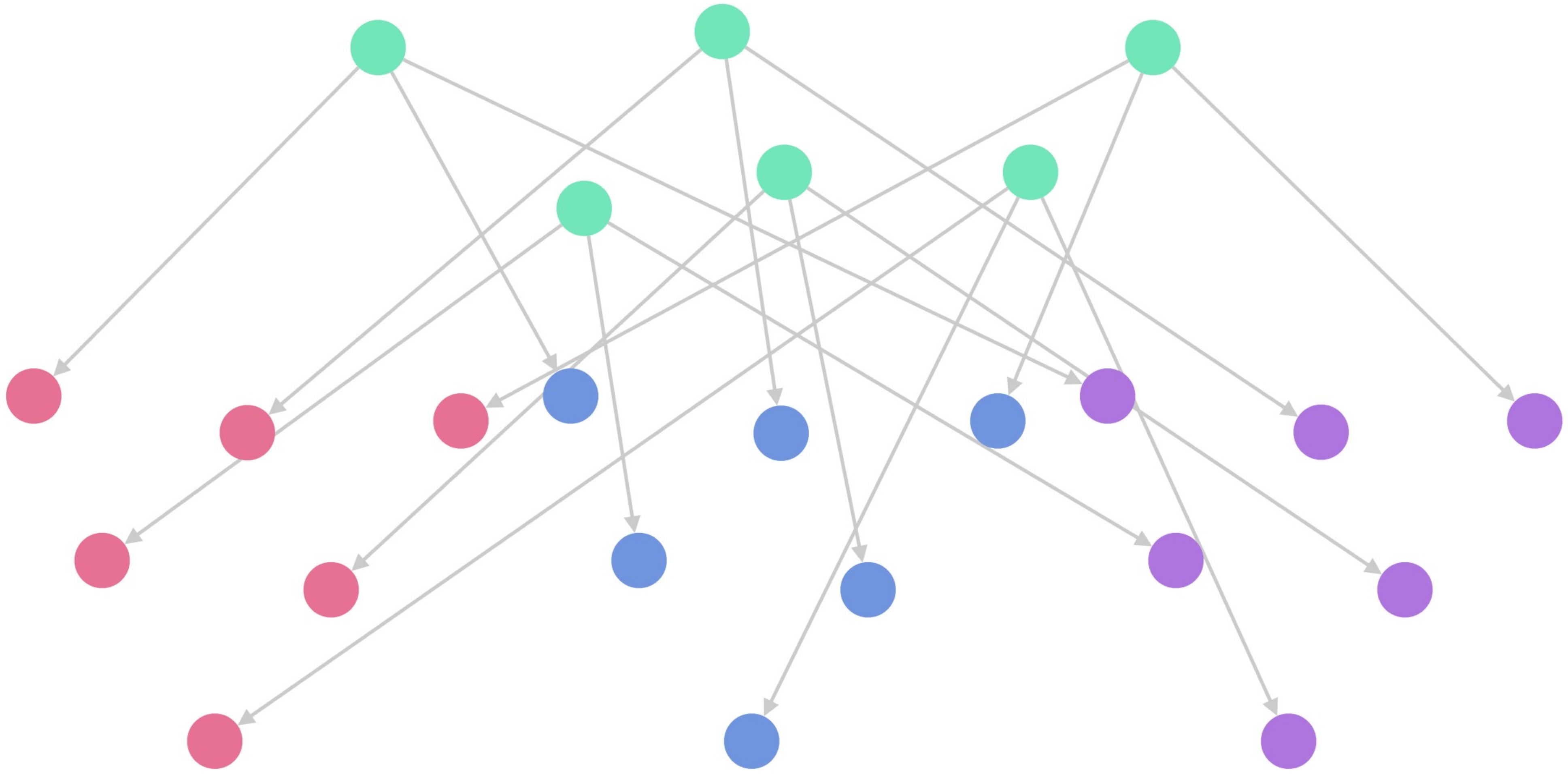


Message Passing Iteration Through the Graph

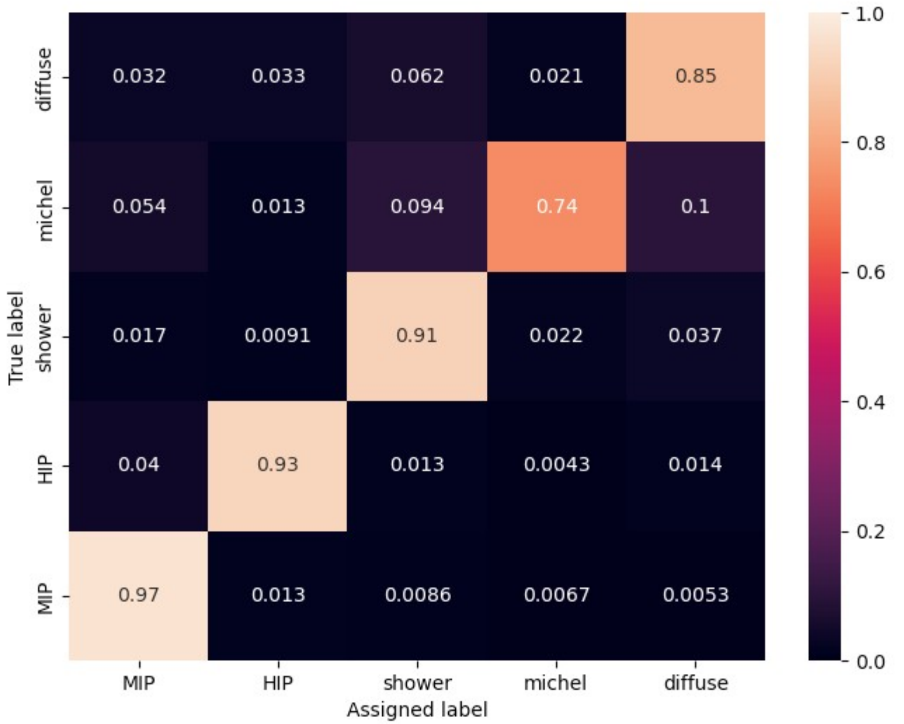
- Propagate 3D nexus node features back down to 2D planar nodes



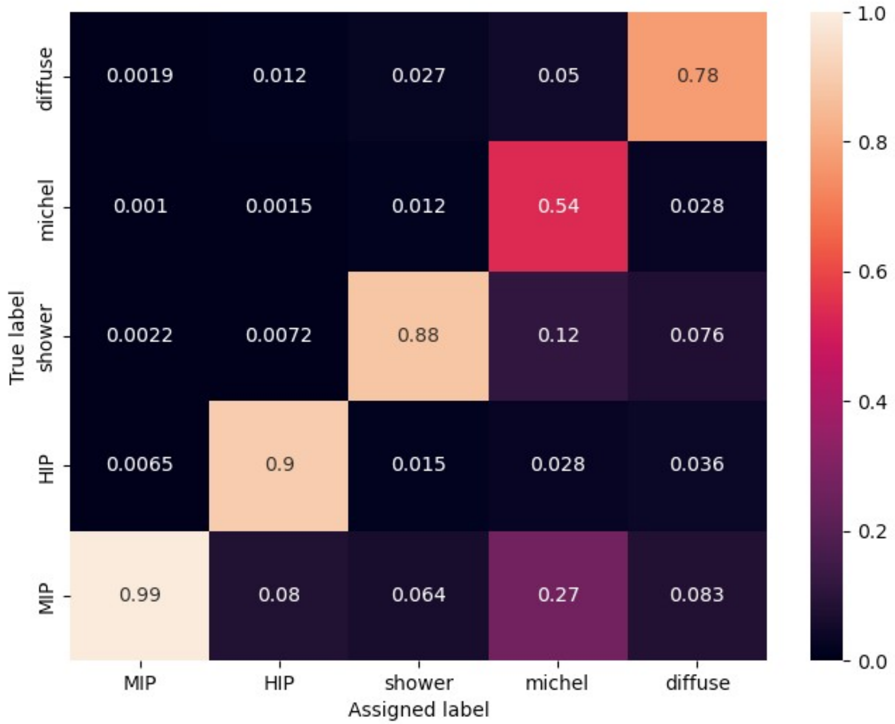
Semantic Hit Classification

- Decoder head trained to classify each hit according to particle type
- Overall efficiency and purity: ~95%
- Consistency between planes ~98%
  - Without 3D nexus connections, ~70% consistency

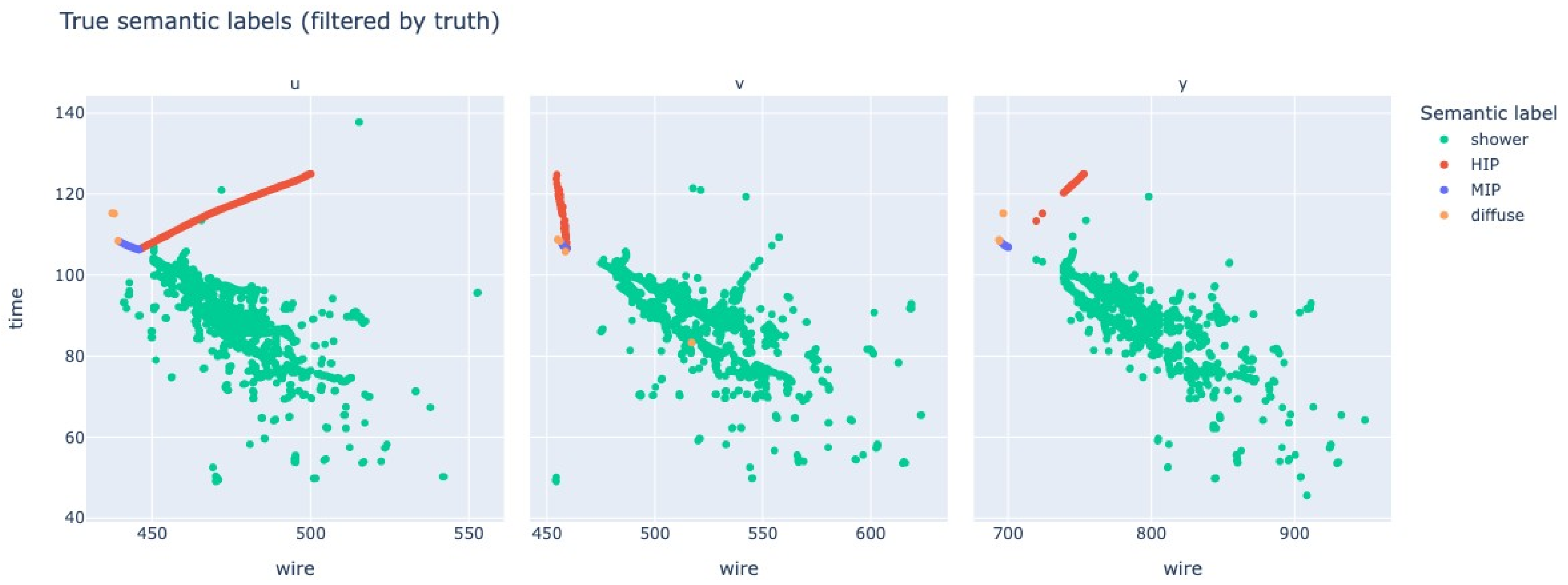
Efficiency



Purity



Event Display: Truth

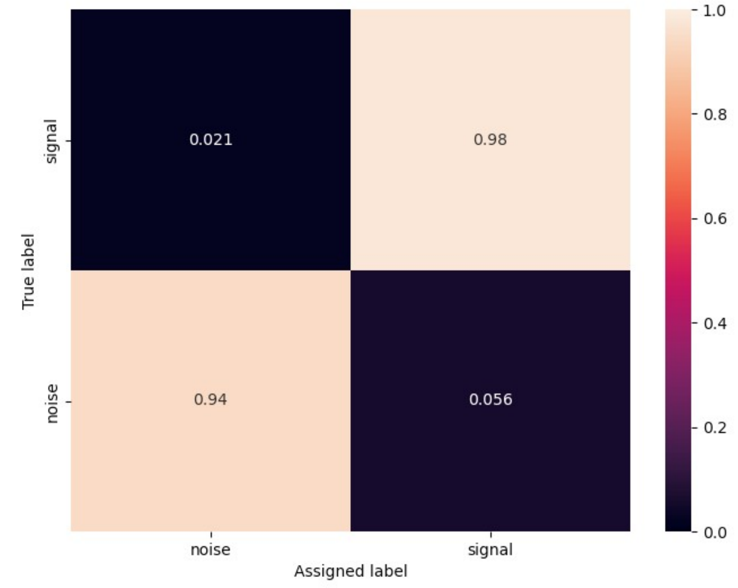


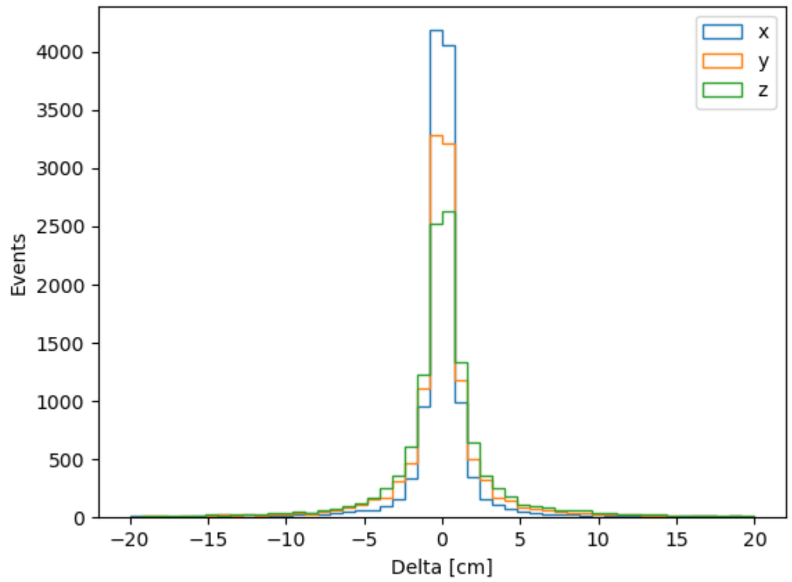
Event Display: Predicted

Auxiliary Tasks

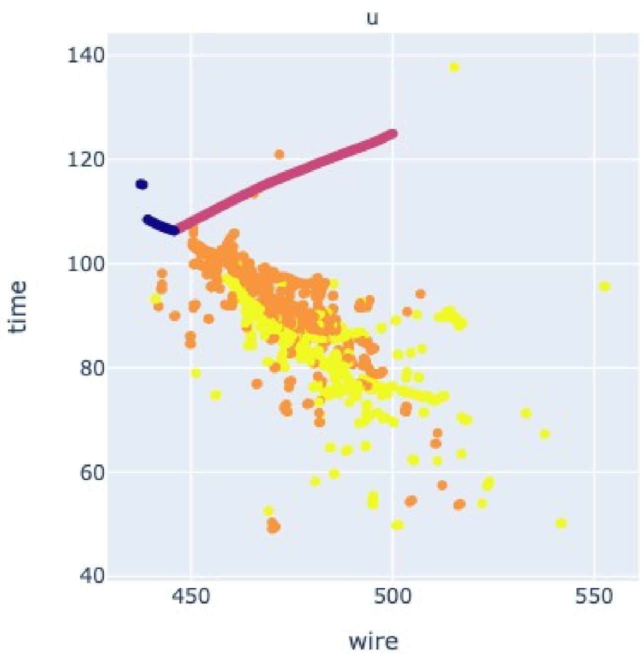
Features produced by NuGraph2 can be fed into separate decoder heads to learn additional tasks

- Cosmic filtering
  - MicroBooNE is on surface ⟶ significant cosmic contamination
  - Train decoder to learn a binary score representing cosmic vs. neutrino
    - Selects neutrino hits with 98% efficiency and purity
- Vertex regression
  - Predict the neutrino interaction vertex position in 3D
  - Currently O(cm) level resolution in each coordinate
- Event classification
  - Classifying full event, similar to NOvA and DUNE CNNs
  - In active development

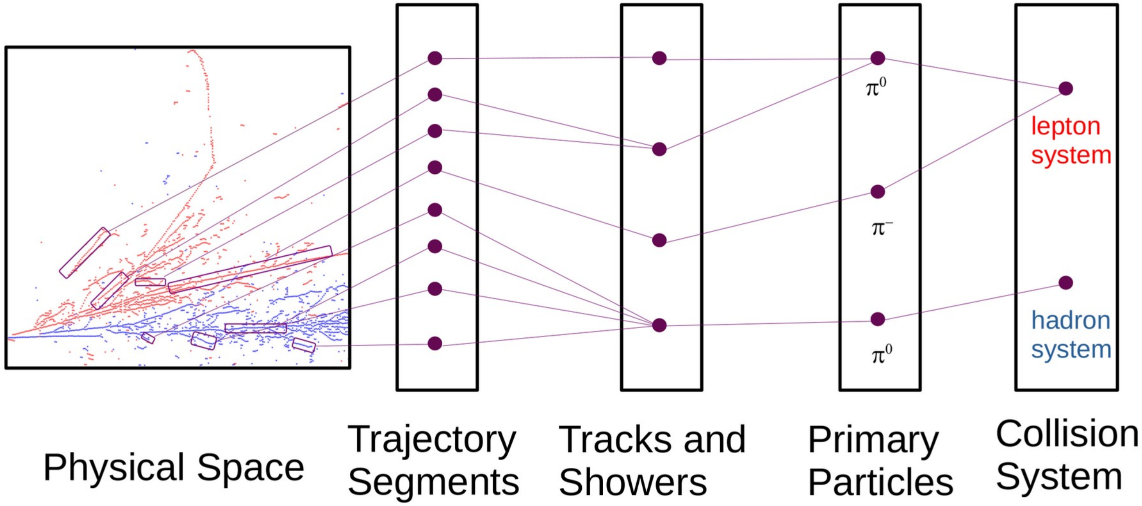




Future



- New decoder head using Object Condensation (arXiv:2002.0306) to group hits into particles
- Share instance labels between planes to group 2D hits into natively 3D clusters



- First pass at clustering will allow for construction of hierarchical graphs
- Second pass hierarchical GNN will refine hypotheses similar to particle flow algorithms

Summary

- NuGraph2 is a multi-purpose GNN architecture for reconstructing neutrino interactions in MicroBooNE
  - Efficiently reject background detector hits
  - Classify detector hits according to particle type
  - Coming soon: vertexing and event classification
- While developed using MicroBooNE open data, it is completely general
  - Already being adapted for DUNE and NOvA
  - Contact us if you think you may have other use cases
- Future work will build towards full reconstruction using hierarchical GNNs

Thank You!